

REPORT DOCUMENTATION PAGE

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Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

21 separate items enclosed

2308M19E

9B

TP- FY99-0084

ERC#E99-003

✓ Spreadsheet
✓ DTS

MEMORANDUM FOR PRS (Contractor Publication)

FROM: PROI (TI) (STINFO)

22 April 1999

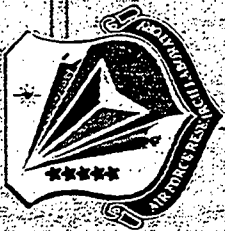
SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-FY99-0084**

Angelo Alfano (ERC), "Decomposition Mechanism and Kinetics Research on Energetic Molecules"

JANNAF

(Statement A)

Best Available Copy



OUTLINE

MOTIVATION

SELECTED APPROACH

DETAILS ON THERMOMETRY FOR GAS PHASE

CONCLUSIONS

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited



New classes of energetic materials (environmental/safety)

- Low vapor pressure solids, ionic liquids
- Little known in advance about their reactive behavior
- Decomposition mechanisms/kinetics needed to incorporate into formulations
- Creates challenging instrumentation requirements
 - Solid, liquid, and gaseous sample formats
 - Transient as well as stable species identification
 - Generalized detection without advance knowledge of identity
 - Kinetics and mechanistic studies at high temperatures
 - Data free of wall-induced reactions



State of the Art

Film heating with rapid scan FTIR

IR laser heating of solid film,
transient trapping, FTIR analysis

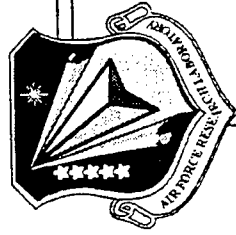
Temperature ramp of few hundred
degrees per second

No kinetic information, no temperature-
time or mechanistic details

Temporal resolution limited
to millisecond regime

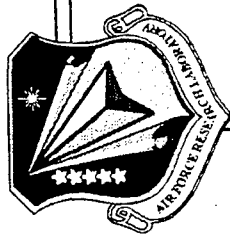
Goals

Combine rapid laser heating with improved temporal resolution
for FTIR analysis and eliminate transient trapping.



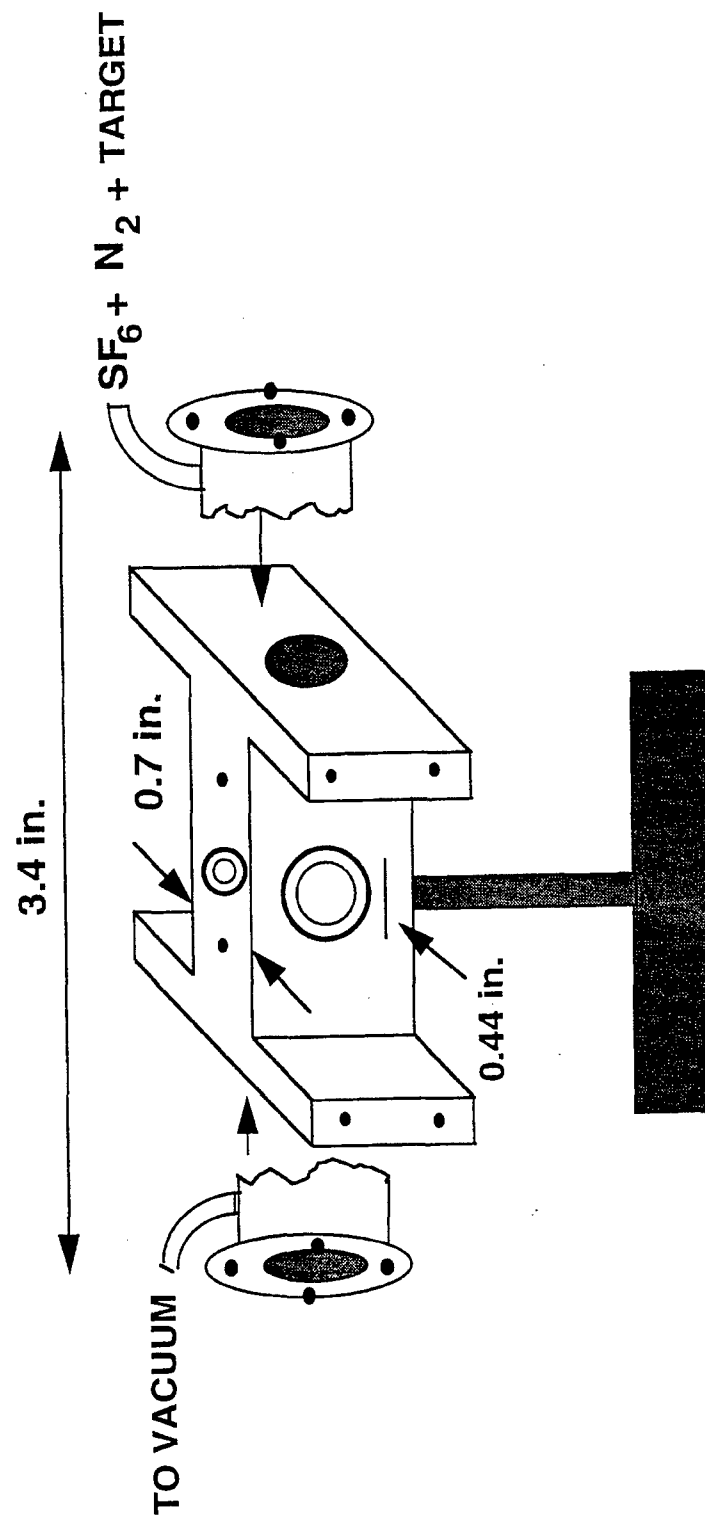
SCOPE OF ISSUES TO BE RESOLVED

- ☐ SENSITIZATION OF SOLIDS AND LIQUIDS AS WELL AS GASES
- ☐ CREATION OF KNOWN STABLE TEMP. FOR KINETICS STUDIES
- ☐ ANY SENSITIZER INDUCED CHEMISTRY?
- ☐ DO PYROLYSIS MECHANISMS CHANGE UNDER THESE CONDITIONS?
- ☐ COUPLING 3 J/PULSE LASER @ 10.6 U WITH SENSITIVE FTIR DETECTOR
- ☐ HOW MUCH TIME AND SAMPLE FOR EXPERIMENT?



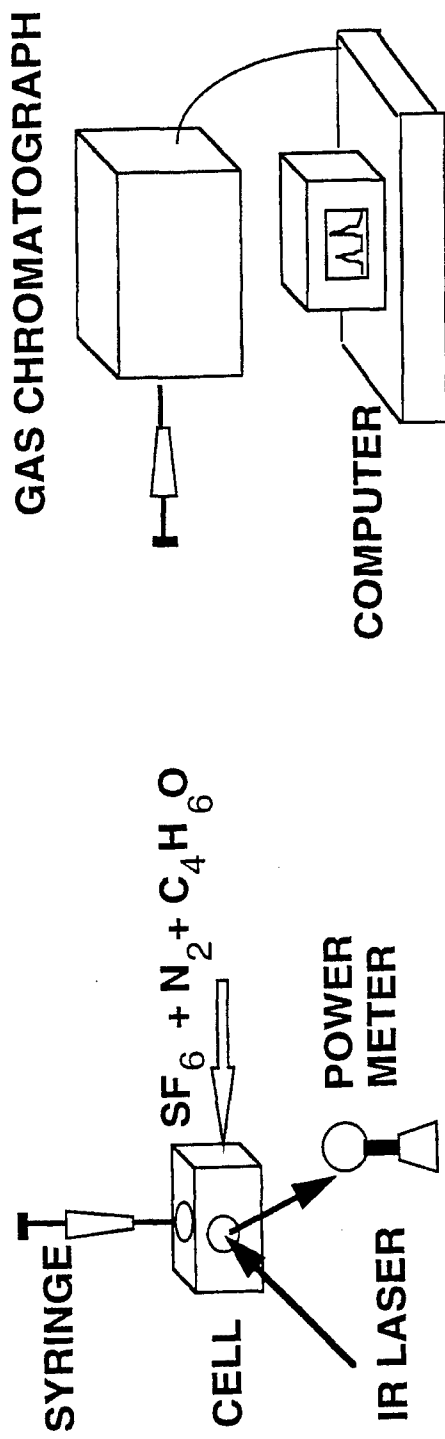
CELL DESIGN CONSIDERATIONS

THIN SAMPLE REGION WITH A LARGE DEAD VOLUME





TEMPERATURE DETERMINATION



$$K_1 = 3.6 \times 10^{14} e^{-52000/RT}$$

+ CO

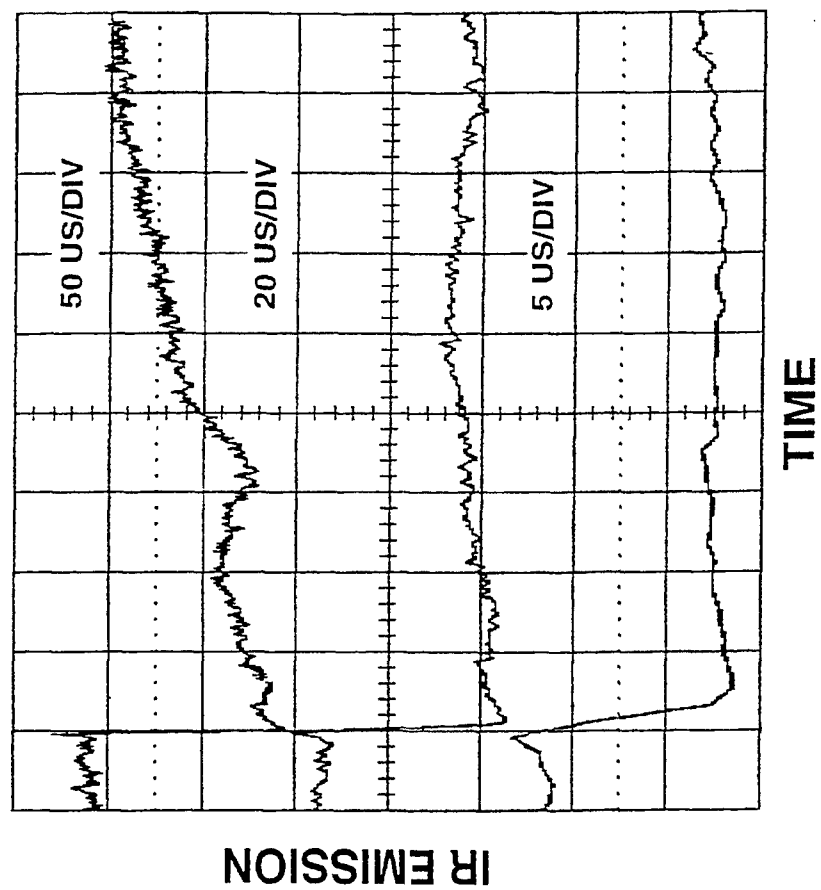
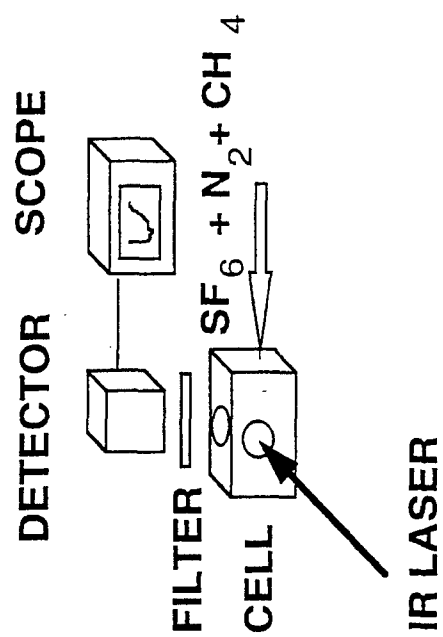


$$K_2 = 2.3 \times 10^{14} e^{-58000/RT}$$

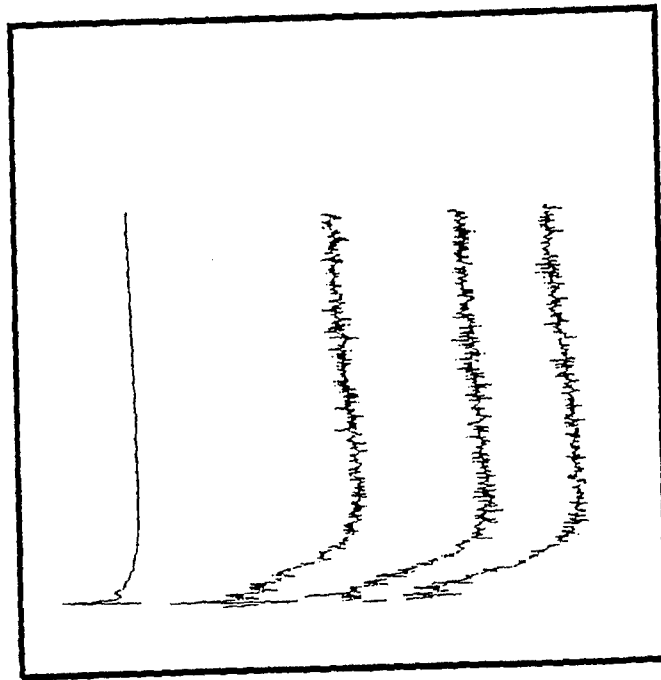
+ C_2H_4



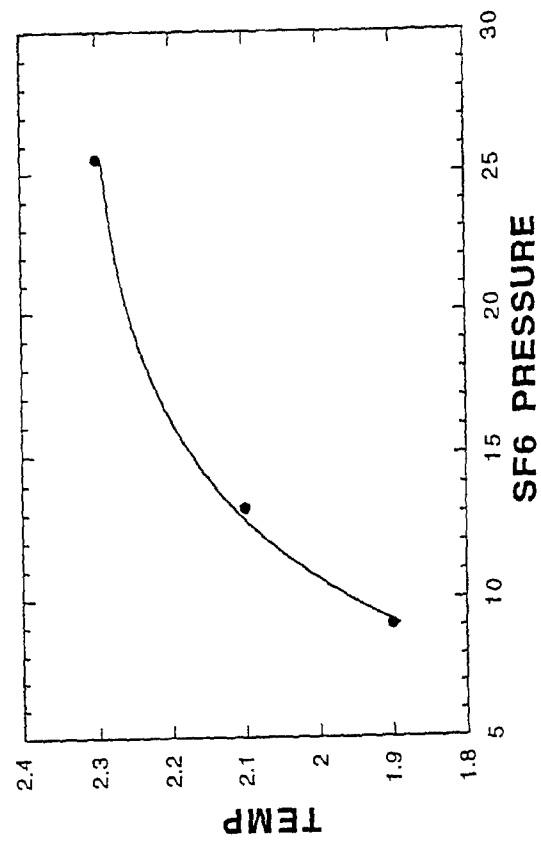
$$T = 1/R (E_{a1} - E_{a2}) / [\ln(A_1/A_2) + \ln(C_2/C_3)]$$

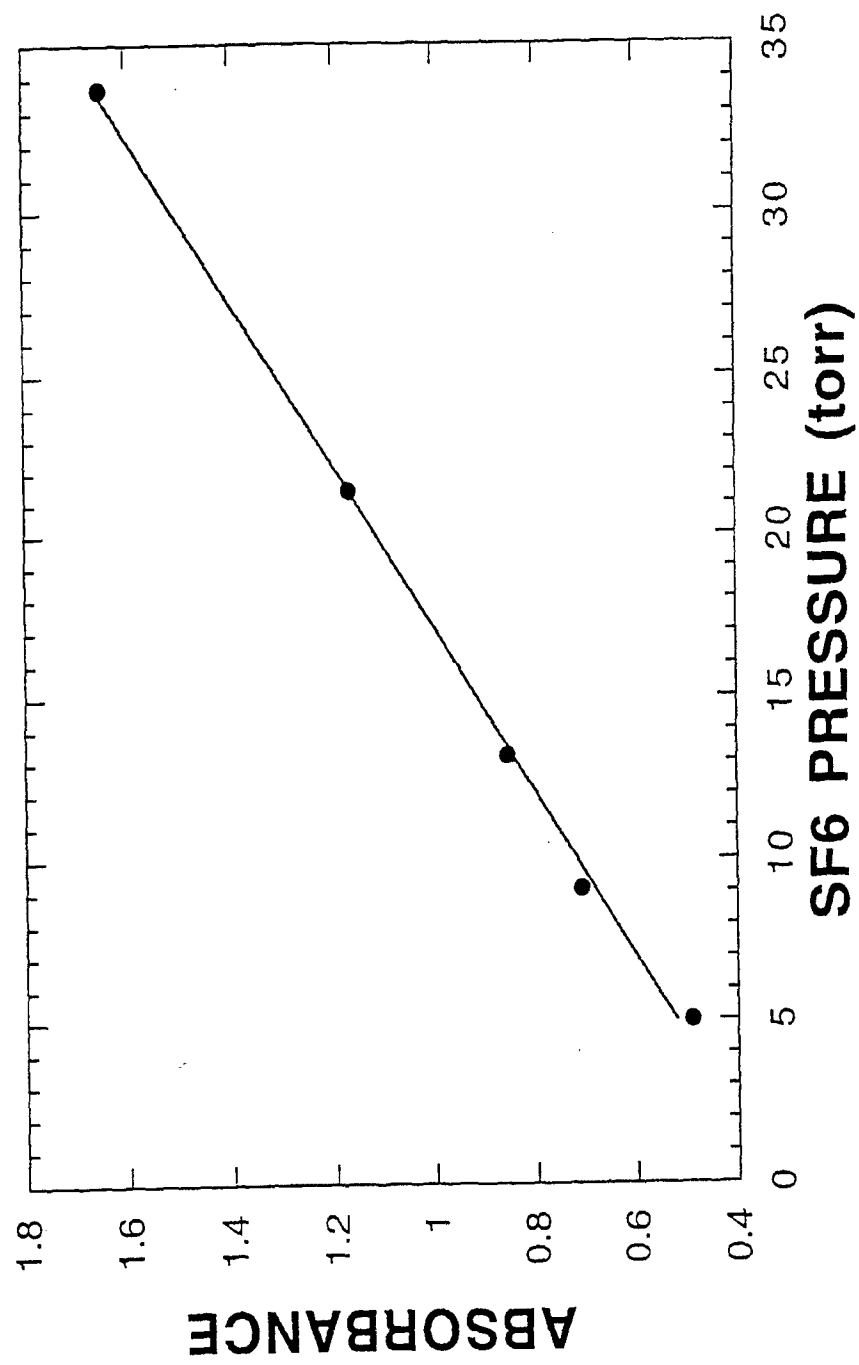


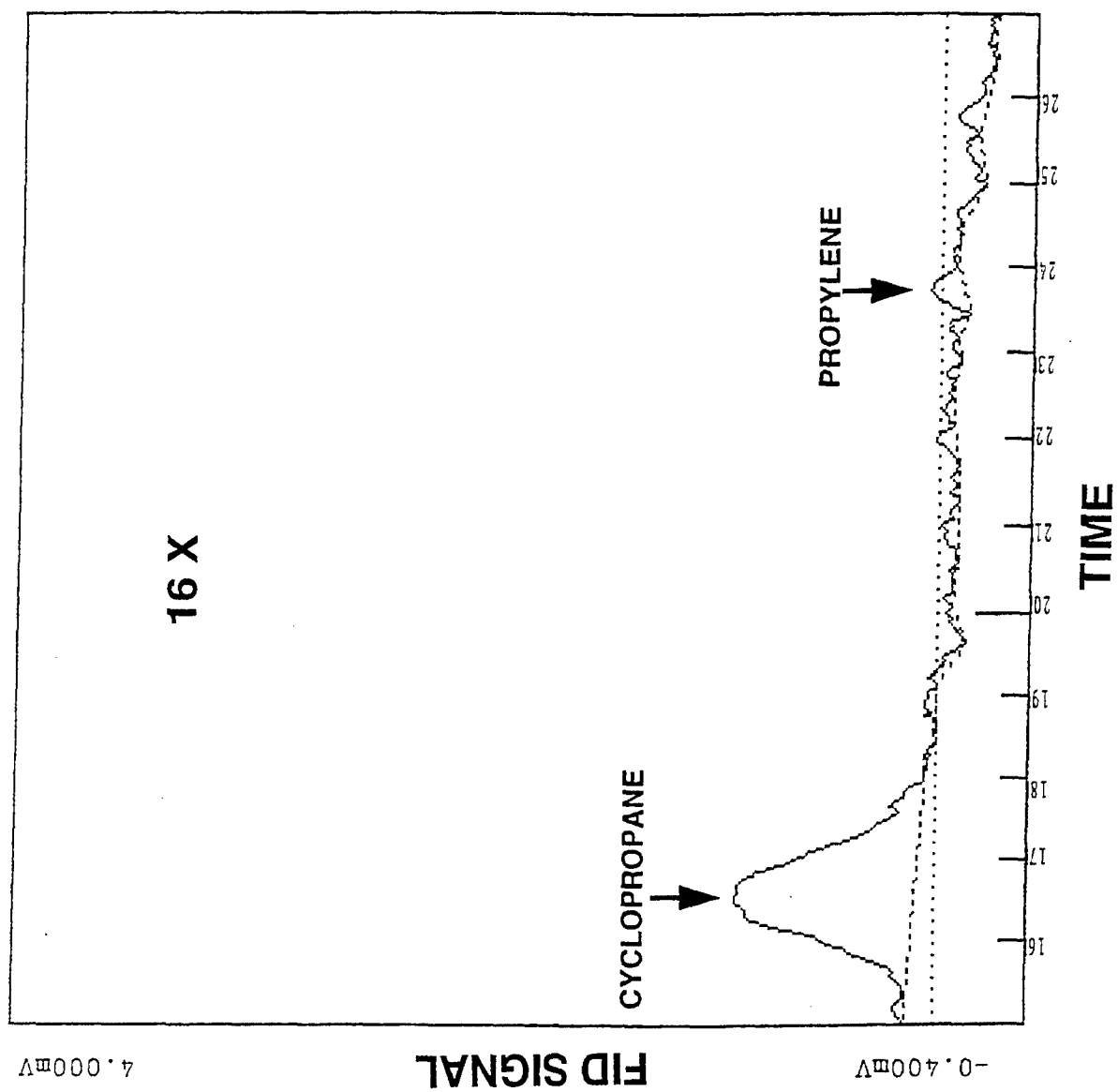
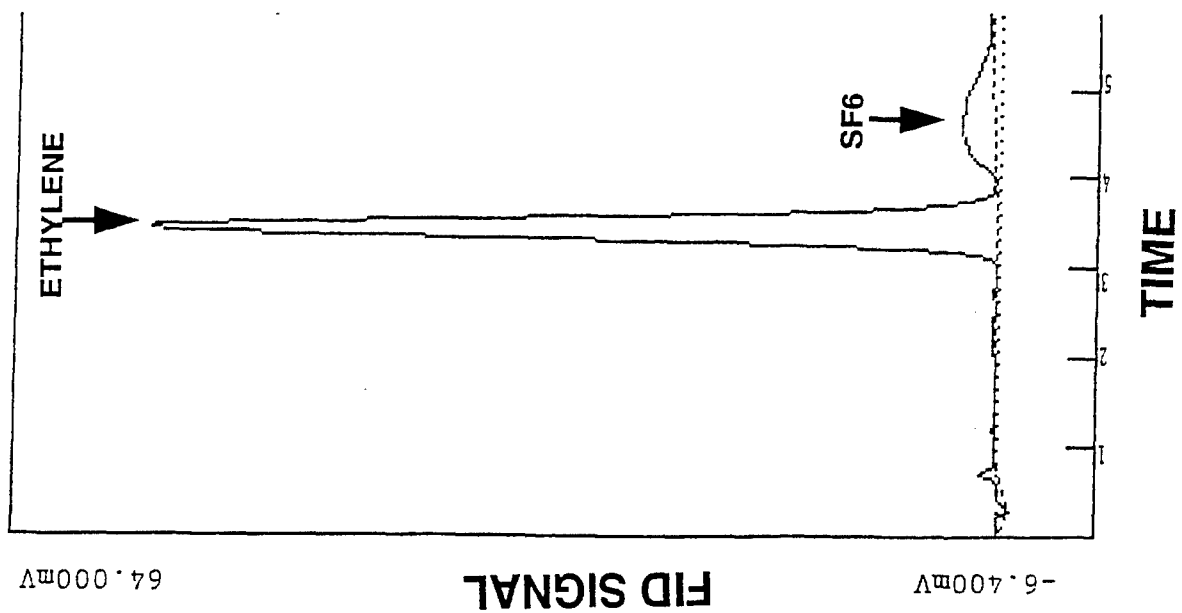
9 MICROSECONDS

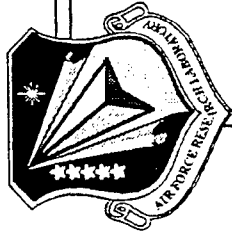


TIME









CONCLUSIONS

- KINETICALLY USEFUL TEMPERATURES IN GAS PHASE
- PULSED IR LASER AND FTIR SEEM COMPATIBLE
- GENERAL TECHNIQUE WITH APPLICATIONS TO HIGH TEMPERATURE MATERIALS, SEMICONDUCTOR PROCESSING, AS WELL AS ENERGETIC MATERIALS

FUTURE

- TRANSIENT IR SPECTRA IN GAS PHASE SAMPLE
- DETAILED SENSITIZATION OF SOLIDS (AND LIQUIDS)